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Modeling multi-element isotope fractionation during biodegradation of organic micropollutants

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Organic micropollutants are often degraded through different reaction pathways. Compound specific isotope analysis is a valuable tool to assess the transformation and to identify degradation pathways of these organic contaminants in different environmental systems. We propose a mechanistic modeling approach that provides a quantitative framework to predict multi-element isotopic evolution during the transformation of different organic micropollutants. The model explicitly simulates the evolution of position-specific isotopologues, containing atoms at isotopically-sensitive positions, and offers mechanistic description of different degradation pathways. The proposed modeling approach is applied to the degradation of three selected organic micropollutants: dichlorobenzamide (BAM), isoproturon (IPU) and diclofenac (DCF). The model successfully reproduces the multi-element isotope data observed in previous experimental studies and precisely captures the dual isotopic trends, characterizing different reaction pathways. Furthermore, the model allows the explicit description of position-specific isotope fractionation as well as primary and secondary isotope effects, which are not always easy to identify and distinguish in experimental studies. Therefore, the approach is useful both for the accurate evaluation of experimental results and as a predictive and design tool to explore degradation scenarios and reaction pathways for which experimental data are not yet available.